3 MATERIALS AND METHODS

3.1 Overview

This project started with the AQUASIM software familiarization. This task was conducted by doing the tutorial that was provided from the supervisor. During doing this task, the related journal paper was reviewed to obtain the parameters to be selected and analysed in the model. After that, a model was developed and the model was run with the selected parameters. Next, the simulation result was compared with the journal result. The developed models were validated so that the model simulation is compatible and produce a good correlation with the experimental data before it can be used for further study. Then, the model was used to study the several scenarios related to operational variability faced by certain industry and the data obtain was analysed.

3.2 Biofilm model, kinetics and parameters

A one-dimensional biofilm model was formed to stimulate the simultaneous nitritation and p-nitrophenol removal using aerobic granular biomass in a continuous airlift reactor performance based on Wanner and Reichert (1996) and applied in the software package AQUASIM (Reichert, 1998),v.2.1d. The reactor volume was set to be fixed at 2.6L based on the experimental data from Jemaat et al, 2013.

The biomass species depicted as particulate compounds in the biofilm matrix were five: ammonia-oxidizing bacteria (AOB), nitrite-oxidizing bacteria (NOB), p-nitrophenol degrader, heterotrophic bacteria, and inert biomass. Biofilm area was designated as a function of the granule radius, to appropriately guess the biofilm geometry. Total biofilm area was expressed as a function of granule size and number of granules. A detachment rate was operated to keep a uniform biofilm thickness in steady state at a predefined value. Detachment biomass from the biofilm was judged as active keep on the same kinetics expressed for the biomass in the biofilm. Attachment of biomass onto the biofilm surface has been ignored. For the sake of easiness external mass transfer has been ignored. The porosity of the biofilm was set as 80% and kept constant throughout the simulation. Initial fraction of particulate compound were 8% AOB,8% NOB, 2% PNP and 2% heterotrophic biomass. The microbial kinetics and the stoichiometry used are detailed in Table 3 and Table 4. Growth of AOB and NOB included inhibition by free ammonia (FA) and free nitrous acid (FNA) as proposed by Jubany et al.,2008 .While, growth of PNP was describe as recently proposed by G.Tziotzios et al, (2008) . Decay of AOB and NOB referring to Munz et al. (2011), with a single rate equation which includes two decay coefficients: a decay coefficient for aerobic and anaerobic condition, which likely will occur in the biofilm and used in the model are detailed in Table 3, and general equation of decay rate is used for decay of PNP.

Table 3: Kinetic parameter

Symbol	Definition	Value	Unit	References
	Ammonium oxidizing bacteria (AOB)			
$\mu_{max,AOB}$	Maximum Specific growth rate of X_{AOB}	2.3	d^{-1}	Jubany et al. (2008)
$b_{AER,AOB}$	Decay rate	0.6	d^{-1}	Munz et al. (2011)
$b_{ANAER,AOB}$	Anaerobic decay rate	0.025	d^{-1}	Munz et al. (2011)
Y_{AOB}	Growth yield	0.18	$gCODg^{-1}N$	Jubany et al. (2008)
$K_{O2,AOB}$	Affinity constant for oxygen	0.74	mgO2/L	Guisasola et al. (2005)
$K_{S,TAN}$	Affinity constant for TAN	11	mgTAN/L	Carrera et al. (2004)
$K_{I,TAN,AOB}$	Inhibition coefficient for TAN	675	mgTAN/L	Jubany et al. (2009)
$K_{I,TNN,AOB}$	Inhibition coefficient for TNN	13115	mgTNN/L	Jubany et al. (2009)
$K_{I,PNP,AOB}$	Inhibition coefficient for PNP	7	$gPNP/m^3$	Jemaat et al.(2013a)
	Nitrite-oxidizing bacteria (NOB)			
$\mu_{max,NOB}$	Maximum Specific growth rate of X_{NOB}	1.65	d^{-1}	Jubany et al. (2008)
$b_{AER,NOB}$	Decay rate	0.25	d^{-1}	Munz et al. (2011)
$b_{ANAER,NOB}$	Anaerobic decay rate	0.012	d^{-1}	Munz et al. (2011)
Y_{NOB}	Growth yield	0.08	$gCODg^{-1}N$	Jubany et al. (2008)
$K_{O2,NOB}$	Affinity constant for oxygen	1.75	mgO2/L	Guisasola et al. (2005)
$K_{S,TNN}$	Affinity constant for TNN	22	mgTNN/L	Ni et al. (2008)
$K_{I,TAN,NOB}$	Inhibition coefficient for TAN	145	mgTAN/L	Jubany et al. (2008)
$K_{I,TNN,NOB}$	Inhibition coefficient for TNN	1431	mgTNN/L	Brockman and Morgenroth (2010)
	***P*-nitrophenol degradation**			
$\mu_{max,PNP}$	Maximum Specific growth rate of X_{PNP}	0.406	d^{-1}	Martín-Hernández et al. (2009)
b_{PNP}	Decay rate	0.212	d^{-1}	Tomei et al.(2004)

Y_{PNP}	Growth yield	0.28	$gCODg^{-1}N$	Martín-Hernández et al. (2009
$K_{O2,PNP}$	Affinity constant for oxygen	1.65	mgO2/L	Jemaat et al. (2013a)
$K_{S,PNP}$	Affinity constant for PNP	1.6	mgPNP/L	Martín-Hernández et al. (2009
$K_{I,PNP}$	Inhibition coefficient for PNP	54	mgPNP /L	Martín-Hernández et al. (2009
		Heterotrophic bacteria (H)		
μ_H	Maximum Specific growth rate of X_H	11.8	d^{-1}	Henze et al. (2000)
b_H	Decay rate	7.87	d^{-1}	Henze et al. (2000)
Y_H	Growth yield	0.67	$gCODg^{-1}N$	Henze et al. (2000)
$K_{O2,H}$	Affinity constant for oxygen	0.2	mgO_2/L	Henze et al. (2000)
$K_{S,S}$	Affinity constant for substrate	4	mgCOD/L	Henze et al. (2000)

Table 4: Diffusivity

Parameter	Symbol	Value	Unit	References
Diffusivity of O_2 in water	D_{O2}	2.2×10^{-4}	m^2d^{-1}	Picioreanu et al.(1997)
Diffusivity of NH4+ in water	D_{TAN}	1.9×10^{-4}	m^2d^{-1}	Picioreanu et al.(1997)
Diffusivity of NO2- in water	D_{TNN}	1.7×10^{-4}	m^2d^{-1}	Picioreanu et al.(1997)
Diffusivity of NO3- in water	D_{NO3}	1.7×10^{-4}	m^2d^{-1}	Picioreanu et al.(1997)
Diffusivity of PNP in water	D_{PNP}	1.7×10^{-4}	m^2d^{-1}	Spigno et al.(2004)
Diffusivity of organic substrate in water	D_S	1.0×10^{-4}	m^2d^{-1}	Picioreanu et al.(1997)
Diffusivity coefficient inside biofilm	E_{Diff}	0.5	Dimensionless	Assumed in the range proposed by Bishop et al.(1995)